Ensemble versus Individual System in Quantum Optics[1]

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Abstract

Modern techniques allow experiments on a single atom or system, with new phenomena and new challenges for the theoretician. We discuss what quantum mechanics has to say about a single system. The quantum jump approach as well as the role of quantum trajectories are outlined and a rather sophisticated example is given.

1. Introduction

Until a decade or so ago only experiments involving *many* atoms were possible, e.g. atoms in an atomic beam or in a gas. With a beam one would have a repetition of measurements on an ensemble, while experiments on atoms in a gas — dilute and with no cooperative effects — can often be viewed as a simu ltaneous measurement on an ensemble.

This is well adapted to the statistical interpretation of quantum mechanics. For the purpose of the present lecture a quantum mechanical expectation value is understood as a *mean value* of measurements on systems of an ensemble, i.e. ensemble averages of an observable or mean square deviations and so on.

With the advent of atom traps, in particular the Paul trap, and with laser cooling it became possible to store a single atom (ion) — or two, three or more — in a trap for hours or days and to experiment with it, e.g. study its interaction with light, microwave radiation or with other atoms. For a single system the statistical interpretation of quantum mechanics, based on ensembles, is not so readily applicable as in the case of beam or a gas. The question we want to address here is the following.

"Does quantum mechanics allow statements for a single system ?"

The answer will be: "Yes, to some extent."

Of course this is trivial if the probability in question is 0 or 1. As a more interesting example of what can happen consider the macroscopic dark periods ('electron shelving') of a *single* three-level atom as proposed by Dehmelt [1]. The atom is supposed to have a ground state 1 and two excited states 2 and $2'$ where the former is strongly coupled to 1 and decays rapidly, while the latter is metastable. The $1-2$ transition is strongly driven by a laser, and the $1-2'$ transition is weakly driven.

Semiclassically the behavior of such a single atom is easy to understand. The electron makes rapid transitions between levels 1 and 2, accompanied by a stream of spontaneous photon emissions, in the order of $10^8 s^{-1}$. These can be detected (and

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even seen by the eye; the stimulated emissions are in the direction of the laser). From time to time the weak driving of the $1 - 2'$ transition manages to put the electron into the metastable level $2'$ where it stays for some time ('shelving'). During this time the stream of spontaneous photons is interrupted and there is a dark period. Then the electron jumps back to level 1 and a new light period begins. In an ensemble of such atoms (e.g. gas with no cooperative effects) light and dark periods from different atoms will overlap, and consequently one will just see diminished fluorescence. Only light and dark periods from a single or a few atoms are directly observable.

In quantum mechanics, however, the atom will always be in a superposition of the three state $|1\rangle$, $|2\rangle$, and $|2'\rangle$ and never strictly in state $|2'\rangle$ for an extended period, i.e. there will always be a small admixture of $|2\rangle$. Since $|2\rangle$ decays rapidly the question arises if the dark periods still occur. Experiments [2] and early theoretical treatment [3] have answered this affirmatively. The duration of the dark periods is random and can be seconds or even minutes.

To treat problems like these involving a single system Wilser and the author [4, 5, 6] developed the quantum jump approach which is equivalent and simultaneous to the Monte-Carlo wave function approach (MCWF) [7] and to the quantum trajectory approach [8]. Our approach is based on standard quantum mechanics and nothing new to the latter is added or required. In the next section we will give a short exposition of the quantum jump approach with its associated random ('quantum') trajectories. In Section 3 we discuss the notion of a spectrum in a light period and of conditional spectra which can be defined for a single fluorescing system. In this case the quantum jump approach leads to more general quantum trajectories.

2. The quantum jump approach. Quantum trajectories

This approach is based on standard quantum mechanics and adds no new assumptions or properties to the latter. In many cases it is just a practical tool for questions concerning a single system and often has technical and conceptual advantages. More details can be found in Refs. [4, 6, 9, 10, 11, 12] and in the recent survey [13].

The underlying idea is that it should make no difference physically whether or not the photons emitted by an atom are detected and absorbed once they are sufficiently far away from the atom. It therefore suggests itself to employ gedanken photon measurements, over all space and with ideal detectors, at instances a time Δt apart[14]. For a single driven atom this may look as in Fig. 1. Starting in some initial state with no photons (the laser field is considered as classical), at first one will detect no emitted photon in space and then at the n_1-th measurement a photon will be detected (and absorbed), the next photon at the n_2-th measurement and so on.

Limits on Δt:

- Ideally one would like to let $\Delta t \to 0$ to simulate continuous measurements. But this is impossible in the framework of standard quantum mechanics with ideal measurements due to the quantum Zeno effect [15].
- Intuitively, Δt should be large enough to allow the photons to get away from

the atom.

- Δt should be short compared to level life-times.

This leads to the requirement [16]

$$\boxed{\Delta t \cong 10^{-13} - 10^{-10} s}$$

To treat these gedanken measurements on a single atom we translate them first into an ensemble description as follows. We consider an ensemble, $\mathcal{E}$, of many atoms, each with its own quantized radiation field, of which our individual atom plus field is a member. At time $t_0 = 0$ the ensemble is described by the state $|0_{ph}\rangle|\psi_A\rangle$. Now we imagine that on each member of $\mathcal{E}$ photon measurements are performed at times $\Delta t, ..., n\,\Delta t, ...$. We consider various sub-ensembles of $\mathcal{E}$:

$$\begin{aligned} \mathcal{E}_0^{(\Delta t)} &\equiv \text{all systems of } \mathcal{E} \text{ for which at time } \Delta t \text{ a photon was detected} \\ \mathcal{E}_0^{(n\Delta t)} &\equiv \text{all systems of } \mathcal{E} \text{ for which at the times } \Delta t, ..., \ n\Delta t \text{ no photon} \\ &\quad \text{was detected (i.e. } \textit{until} \text{ time } n\Delta t \text{ no photon!)} \end{aligned}$$

This is depicted in Fig. 2 where our individual system, atom plus radiation field, is denoted by a dot $\cdot$, and it is a member of $\mathcal{E}_0^{(n\Delta t)}$ for $n < n_1$.

Now one can proceed by ordinary quantum mechanics and the von Neumann-Lüders reduction rule [17]. Let $\mathcal{P}_0$ be the projector onto the no-photon subspace,

$$\mathcal{P}_0 \equiv |0_{ph}\rangle \mathbf{1}_A \langle 0_{ph}| \tag{1}$$

and let $U(t, t_0)$ be the complete time-development operator, including the laser driving and the interaction of the atom with the quantized radiation field. Then the sub-ensemble $\mathcal{E}_0^{(\Delta t)}$ is described by

$$\mathcal{P}_0 U(\Delta t, 0)|0_{ph}\rangle|\psi_A\rangle \tag{2}$$

and the sub-ensemble $\mathcal{E}_0^{(n\Delta t)}$ by

$$\mathcal{P}_0\, U(n\Delta t, (n-1)\Delta t)\mathcal{P}_0 ... \mathcal{P}_0\, U(\Delta t, 0)|0_{ph}\rangle|\psi_A\rangle \equiv |0_{ph}\rangle|\psi_A \underbrace{(n\Delta t)}_{\equiv t}\rangle\ . \tag{3}$$

The relative size of the sub-ensemble $\mathcal{E}_0^{(n\Delta t)}$ is the probability to find a member of $\mathcal{E}$ in $\mathcal{E}_0^{(n\Delta t)}$ and is given by the norm-squared of the above expression. Hence

$$\begin{aligned} P_0(t) &\equiv \| \, |\psi_A(t)\rangle \|^2 \\ &= \text{probability to find no photon until } t = n\Delta t \end{aligned} \tag{4}$$

To calculate $|\psi_A(t)\rangle$ we note that

$$\mathcal{P}_0\, U(t' + \Delta t, t')\mathcal{P}_0 = |0_{ph}\rangle\langle 0_{ph}|U(t' + \Delta t, t')\,|0_{ph}\rangle\langle 0_{ph}| \tag{5}$$

and that the inner expression is a purely atomic operator which is easily obtained by second order perturbation theory. For Δt in the above limits one then obtains, on a

coarse-grained time scale (for which Δt is very small), that the time-development of $|\psi_A(t)\rangle$ is given by a 'conditional', or 'reduced', non-Hermitian Hamiltonian $H_{\rm cond}$ in the atomic Hilbert space where, for an N-level atom,

$$H_{\rm cond} = H_A(t) - i\hbar\Gamma \tag{6}$$

with $H_A(t)$ the atomic part of the Hamiltonian, including the laser driving, and

$$\Gamma \equiv \sum_{\substack{\alpha i j \\ \alpha<i,j}} \Gamma_{i\alpha\alpha j}|i\rangle\langle j| \tag{7}$$

$$\Gamma_{ijlm} \equiv e^2\langle i|\mathbf{X}|j\rangle\cdot\langle|\mathbf{X}|m\rangle\,|\omega_{lm}|^3/(6\pi\epsilon_0\hbar c^3) \tag{8}$$

and $e\mathbf{X}$ the dipole operator. Γ consists of generalized damping terms, and we note that

$$\Gamma_{i\alpha\alpha i} \equiv \Gamma_{i\alpha} \ = \frac{1}{2}A_{i\alpha}$$

where $A_{i\alpha}$ is the Einstein coefficient for the transition from level i to level α. Thus, on a coarse-grained time scale, one obtains

$$|\psi_A(t)\rangle = \mathcal{T}\exp\{-i\int_0^t dt' H_{\rm cond}(t')/\hbar\}|\psi_A(0)\rangle \tag{9}$$

$$\equiv U_{\rm cond}(t,0)|\psi_A(0)\rangle\ . \tag{10}$$

In an obvious extension to density matrices,

$$\rho_A^0(t) \equiv U_{\rm cond}(t,0)\rho_A(0)U_{\rm cond}(t,0)^\dagger \tag{11}$$

describes the sub-ensemble with no photon detection until time t, with the corresponding no-photon probability given by

$$P_0(t) = {\rm tr}\rho_A^0(t)\ . \tag{12}$$

If one lets $\Delta t \to 0$ in Eq. (3), with $t = n\Delta t$ kept fixed, then one easily sees by the same calculation that the probability to find no photon until time t goes to 1 and that one always stays in the no-photon subspace. This means that for $\Delta t \to 0$ the dynamics is frozen to the atomic subspace, and this is a particular form of the quantum Zeno effect.

A single fluorescent atom as a sample path: Quantum trajectories

Now we can return to the gedanken measurements on our single atom driven by lasers. We can distinguish different steps in its temporal behavior.

- Until the detection of the first photon, our atom belongs to the sub-ensembles $\mathcal{E}_0^{(n\Delta t)}$ and hence is described by the (non-normalized) vector

$$|\psi_A(t)\rangle = U_{\rm cond}(t,0)|\psi_A(0)\rangle. \tag{13}$$

- The first photon is detected at some (random) time t_1, according to the probability density

$$w_1(t) = -\frac{dP_0(t)}{dt} = -\frac{d}{dt}\| \, |\psi_A(t)\rangle \|^2 \; . \tag{14}$$

- *Jump:* With the detection of a photon the atom has to be reset to the appropriate state. For example a two-level atom will be in its ground state right after a photon detection. The general reset state has been determined in Refs. [6, 12] and it may depend on $|\psi_A(t_1)\rangle$ where t_1 is the detection time.

- From this reset state the time development then continues with $U_{\rm cond}(t, t_1)$, until the detection of the next photon at the (random) time t_2. Then one has to reset (jump), and so on.

In this way one obtains a

stochastic path in the Hilbert space of the atom.

The stochasticity of this path is governed by quantum theory, and the path is called a *quantum trajectory*. The stochastic process underlying these trajectories is a jump process with values in a Hilbert space. If the reset state is always the same, e.g. the ground state, one has a renewal process. If the reset state depends on $|\psi_A(t_i)\rangle$ one has a Markov process only.

As shown in Ref. [6] the ensemble of all possible trajectories obtained in this way leads to a reduced density matrix for the ensemble of atoms which satisfies the usual optical Bloch equations. This is a nice consistency check [22].

In case of a renewal process the parts of a trajectory between jumps behave like an ensemble created by *repetition* from a single system at stochastic times. In the general case the reset states can all be different so that this repetitive property is no longer true.

Observables for a single system

Since the individual photon detection times for a single driven atom are random, they cannot be predicted. However, time averages along a trajectory are more promising, e.g. the mean distance between two subsequent photon detections or other correlations.

If the underlying stochastic process is *ergodic* then

time average over a single trajectory = ensemble average

and this equality allows easy calculation. In many cases, e.g. for a renewal process, ergodicity is easy to see. We believe that it is probably true in general for the quantum trajectories[18].

Hence for *observables such as time averages quantum mechanics allows predictions for single systems*. As applications we mention macroscopic dark periods [4, 9] and quantum counting processes [6] where the axioms introduced by Davies and Srinivas [19] are not needed.

There is a word of caution, however. For the observable "frequency spectrum of fluorescent radiation" from a single atom the above trajectories are not (directly) applicable. This has to do with the time-energy uncertainty relation. If all photon detection times were known by measurements then the spectrum would be broadened and deformed. This shows that the above quantum trajectories are not "realistic" and should therefore not be over-interpreted. They are just a useful quantum mechanical tool in certain situations. There is also a relation with the consistent-histories approach to quantum mechanics [20].

3. A surprising example. More general quantum trajectories

Sometimes it is advantageous to carry over the quantum jump approach to a situation where one asks more general questions about the temporal behavior of a single system subject to observations. To motivate this we return to the light and dark periods of the Dehmelt system mentioned in the Introduction. The light and dark periods are depicted in Fig. 3. The semiclassical considerations of the Introduction suggest that the light periods are mainly due to transitions between levels 1 and 2. Now the frequency distribution of light emitted by a laser-driven two-level system is given by the Mollow spectrum. For weak driving this consists of a Lorentzian spectrum around the laser frequency ω_L ("incoherent part") plus a δ peak (Rayleigh peak, "coherent part") at ω_L. For strong driving the incoherent part consists of three Lorentzian parts (Mollow triplet).

Complete spectrum: Let us now turn to the frequency spectrum emitted by the three-level Dehmelt system and use some simple arguments to see what to expect. *Classically,* the δ or Rayleigh peak of the two-level system would correspond to the emission of an electromagnetic field with sharp frequency ω_L. For the three-level case the amplitude of this field is zero during the dark periods, and hence classically one would have an amplitude-modulated signal. From radio engineering one knows that classical amplitude-modulated signals contain sidebands. Because the dark periods have random lengths the sidebands should be continuous and should lead to a partial broadening of the δ or Rayleigh peak. Surprisingly, this is exactly what the fully quantum mechanical calculation predicts [21], and the result is given in Fig. 4. On top of the center of the Mollow spectrum there is an additional narrow Lorentzian peak, and then the Rayleigh peak. This is the spectrum from an ensemble of such atoms, or from a single atom whose light emitted from time zero to infinity is spectrally analyzed. For this spectrum one can show that there is no difference between ensemble and single system, due to ergodicity. Fig. 5 shows the enlarged center of the spectrum for a different set of parameters.

By the classical analogy, more frequent dark periods should mean more modulation and should thus lead to a wider broadening of the Rayleigh peak. The quantum mechanical calculation again confirms this expectation.

Spectrum for single system in a light period: Taking the classical explanation one

step further would clearly imply:

$$\boxed{\text{spectrum in a light period} \neq \text{complete spectrum}}$$

Remarks

- If at all, the notion of spectrum in a light period can only be meaningful for a *single* system!
- The time-frequency uncertainty relation will of course introduce a broadening. The light period under consideration should therefore be so long that this broadening is negligible.
- How does one know one is in a light period? By photon counting. But this disturbs the spectrum, by the time-energy uncertainty relation, as explained in Section 2! So how to measure the spectrum without disturbing it?

To overcome the last objection to a proper quantum mechanical notion of the spectrum in a light period, we suggested in Ref. [21] the setup depicted in Fig. 6. A laser-driven atom emits radiation. In the right half-space an ideal broadband photodetector registers all photons and triggers a spectrometer (spectral analyzer) in the following way. A light period in the right half-space is defined as a sequence of photon detections whose temporal distance in less than some prescribed time T_0. A dark period is a time interval which is longer than T_0 and with no detection occurring. Now the broadband counter in the right half-space opens the spectral analyzer in the left half-space at the beginning of a light period and closes it at the end (after an additional time T_0, to be precise). All data for light periods in the right half-space of length less than some prescribed T are discarded. In this way one obtains a sequence of spectral data for the left half-space referring to light periods in the right half-space of length at least T. The spectral data for individual light periods may depend on the actual detection pattern for the photons in the right half-space and one can average over these. The notion of spectrum outlined above may be properly called a conditioned or *conditional spectrum* because one performs a selection of spectral data based on prescribed conditions.

Generalized quantum trajectories: To calculate this conditional spectrum in a light period we have generalized the above quantum jump approach and its quantum trajectories in a natural way, adapted to the problem at hand [21]. At a no-photon detection in the right half-space the state is not projected with the projector $\mathcal{P}_0$ of Eq. (1) onto the global no-photon subspace, but rather onto those no-photon states belonging to modes with momenta in the right half-space. The resulting projected state will contain, in addition to an atomic part, also photon modes with momenta in the left half-space. This leads to a more complicated time development between detections. Once a photon has been detected and absorbed in the right half-space one has to reset the state (a "jump"). The jump in general leads to a density matrix involving the atoms and photons from the left half-space. In this way one obtains a quantum trajectory consisting of density matrices where the latter simultaneously describe the atom together with a subset of modes of the radiation field.

This generalized quantum jump approach has been used to calculate the conditional spectrum in a light period [21]. As expected the broadening of the Rayleigh peak disappears. For the same parameters as in Fig. 5 the dotted curve in Fig. 7 shows the corresponding spectrum in a light period which is long enough so that the broadening of the Rayleigh peak due to the time-frequency uncertainty relation is negligible. Of course, with increasing length such light periods become very rare. To define a light period we have chosen $T_0 = 50\Gamma_{22}^{-1}$, and so classically a light phase can still have some amplitude modulation. This explains the small bump in the line center.

The above example is in several respects amazing. First of all, quite elementary classical arguments about radiation from driven atoms turn out to be qualitatively correct (to a large extent also quantitatively so, cf. Ref. [21]), although the quantum solution is much more complicated. Furthermore, it shows that there are interesting questions concerning a single system which at first sight seem contradictory but still allow a quantum theoretical treatment.

4. Conclusions

The usual statistical interpretation of quantum mechanics uses the ensemble point of view. In this view a state vector or density matrix describes not a single system but an ensemble of identically prepared systems. Nevertheless, it is sometimes useful to ascribe a state $|\psi\rangle$ or density matrix ρ also to a single system. By this we mean that the system is prepared by the same apparatus as that for the corresponding ensemble.

In this lecture we have tried to convey several points.

- Experiments with a single system (atom, ion) show phenomena which are absent for an ensemble (e.g. in a gas with no cooperative effects).
- A convenient tool for a description of such experiments with a single system is often given by the quantum jump approach with its (random) quantum trajectories. This approach is based on standard quantum mechanics and does not go beyond it.
- The quantum jump approach is useful for questions related to the statistics of photons emitted from a single system. More general problems, like the frequency spectrum in a light period, require more general trajectories.
- The set of quantum trajectories for a driven atom give the reduced density matrix equations (optical Bloch equations) for the ensemble of atoms.
- Since quantum trajectories are adapted to the particular problem under consideration a quantum trajectory is not a "realistic" property of a single system. Rather, the complete information is contained in the state vector (or density matrix) of the system plus radiation field.

An interesting question relating to ergodicity was touched upon in the text. Are time averages independent of the particular quantum trajectory? Or could they vary

for different individual systems? That they do not is usually assumed in experiments. Is this always true or does one need additional assumptions?

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[15] As will be pointed out further below, the calculation of the photon emission probabilities will automatically give zero for the present case when $\Delta t \to 0$. This is a special manifestation of the quantum Zeno effect. Extensive references on this effect can be found in A. Beige and G.C. Hegerfeldt, Phys. Rev. A **53** (1996) and in A. Beige, G.C. Hegerfeldt, and D.G. Sondermann, Found. Physics (Dec. 1997, in press).

[16] For a similar requirement cf. P.A.M. Dirac, *The Principles of Quantum Mechanics*, 4th Ed., Clarendon Press (Oxford 1959), p. 181.

[17] The projection postulate as commonly used nowadays is due to G. Lüders, Ann. Phys. **8**, 323 (1951). For observables with degenerate eigenvalues his formulation differs from that of J. von Neumann, *Mathematische Grundlagen der Quantenmechanik*, Springer (Berlin 1932) (English translation: *Mathematical Foundations of Quantum Mechanics*, Princeton University Press, 1955), Chapter V.1. The projection postulate intends to describe the effects of an ideal measurement on the state of a system, and it has been widely regarded as a useful tool. Cf. also the remark in P.A.M. Dirac, *The Principles of Quantum Mechanics*, 1st Ed., Clarendon Press (Oxford 1930), p. 49, about measurements causing minimal disturbance. In later editions this passage has been omitted.

[18] It would indeed be very interesting if there were non-ergodic quantum trajectories. Then there could be different time averages for different trajectories.

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Figure Captions

Fig. 1: Repeated photon measurements.

Fig. 2: Ensemble $\mathcal{E}$ and sub-ensembles. The dot denotes our single system.

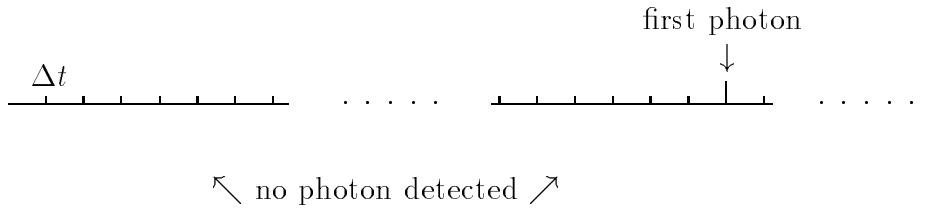
Fig. 3: The light periods consist of rapid sequences of photon emissions.

Fig. 4: Frequency spectrum with an additional narrow Lorentzian peak due to dark periods ($\Delta \equiv \omega - \omega_L$).

Fig. 5: Enlarged center of spectrum for a different set of parameters ($\Delta \equiv \omega - \omega_L$).

Fig. 6: The broadband photo-detector in the right half-space triggers the spectrometer in the left half-space during a long light period.

Fig. 7: Dotted line: The narrow Lorentzian peak of Fig. 5 is absent in a long light period ($\Delta \equiv \omega - \omega_L$).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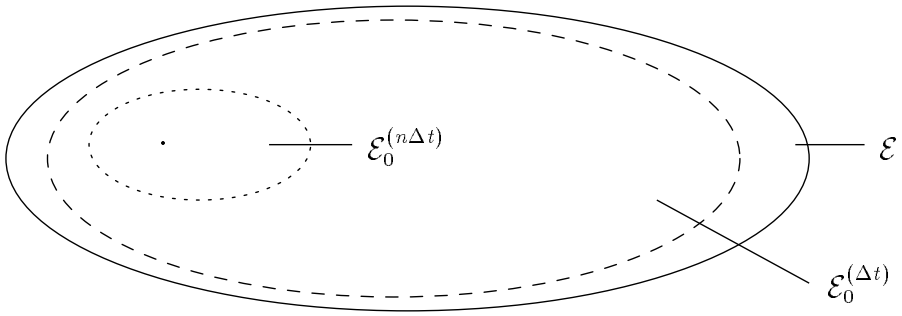
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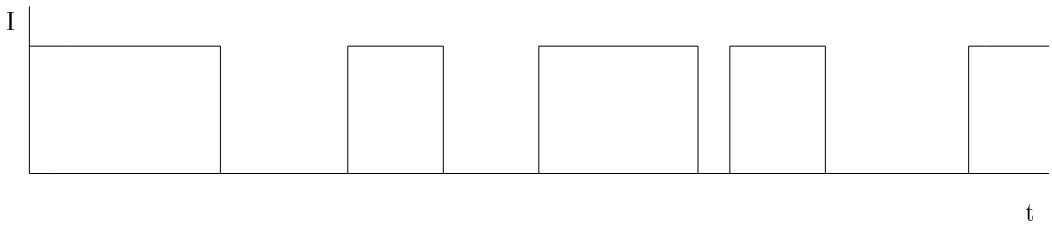
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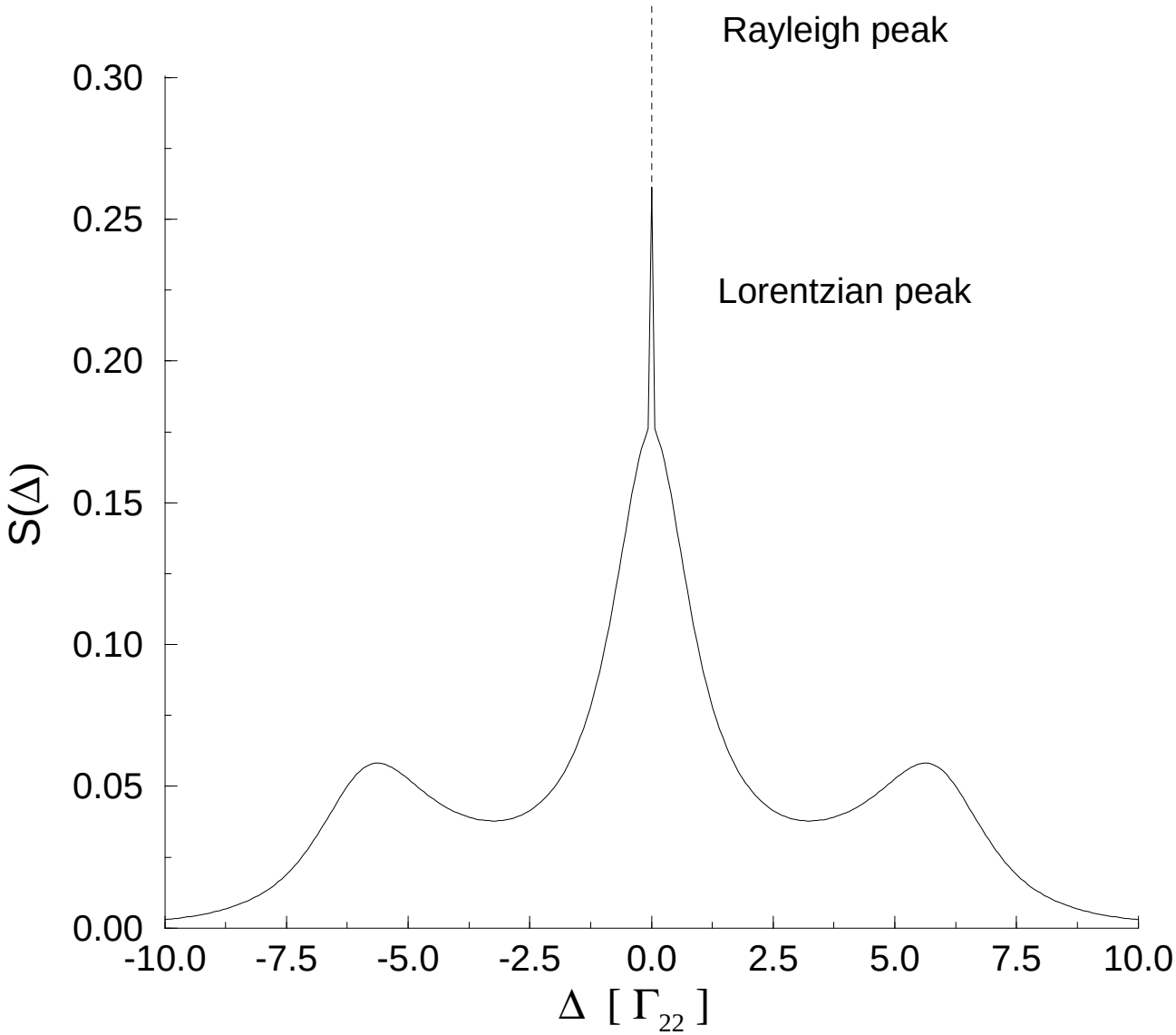
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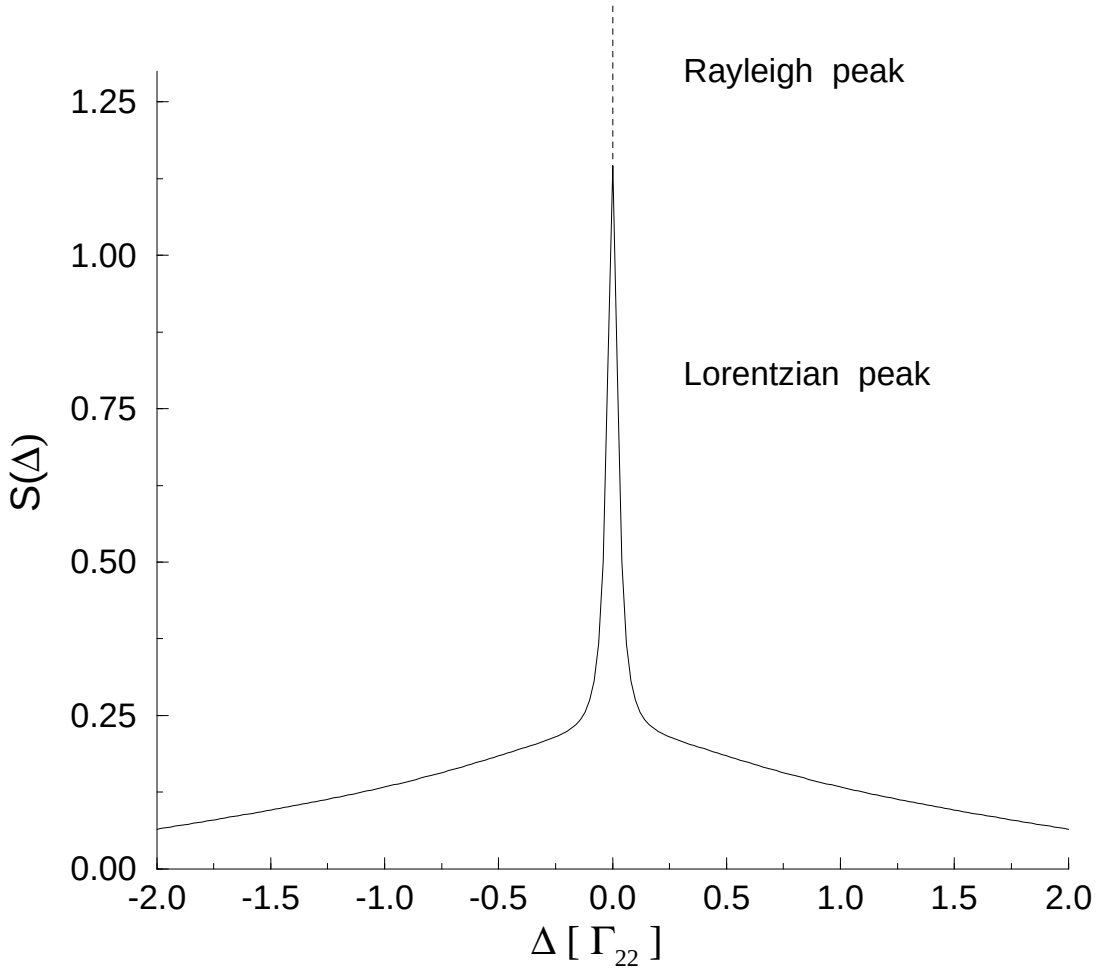
Δ [Γ22]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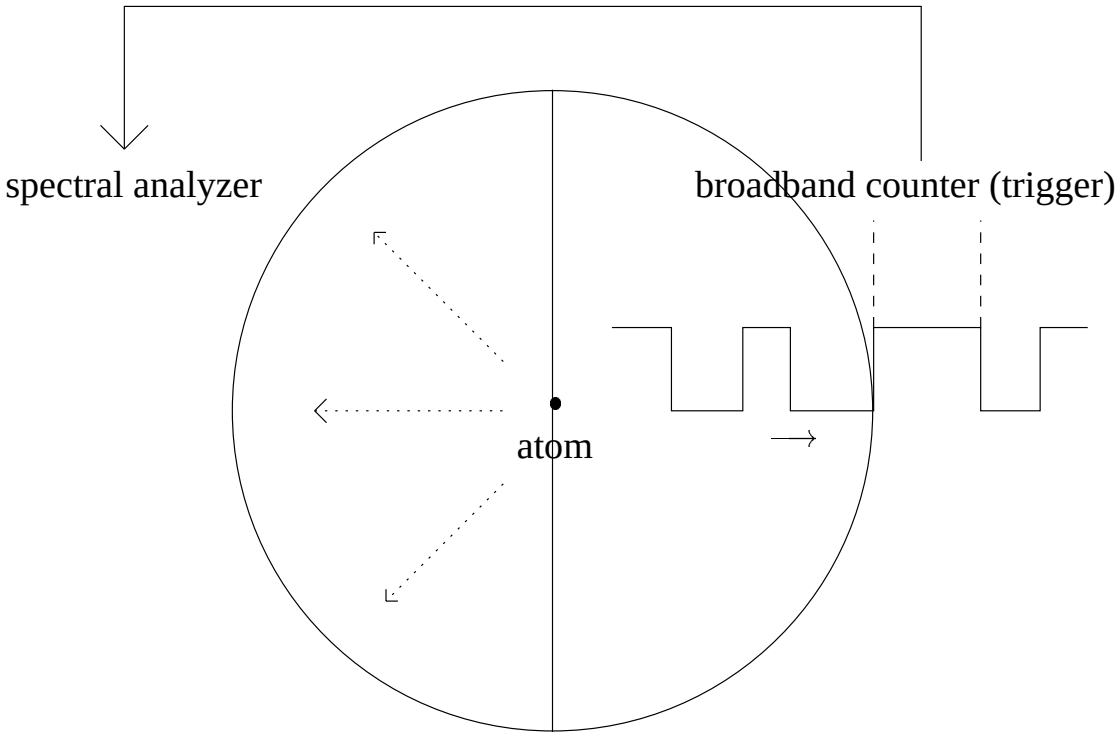
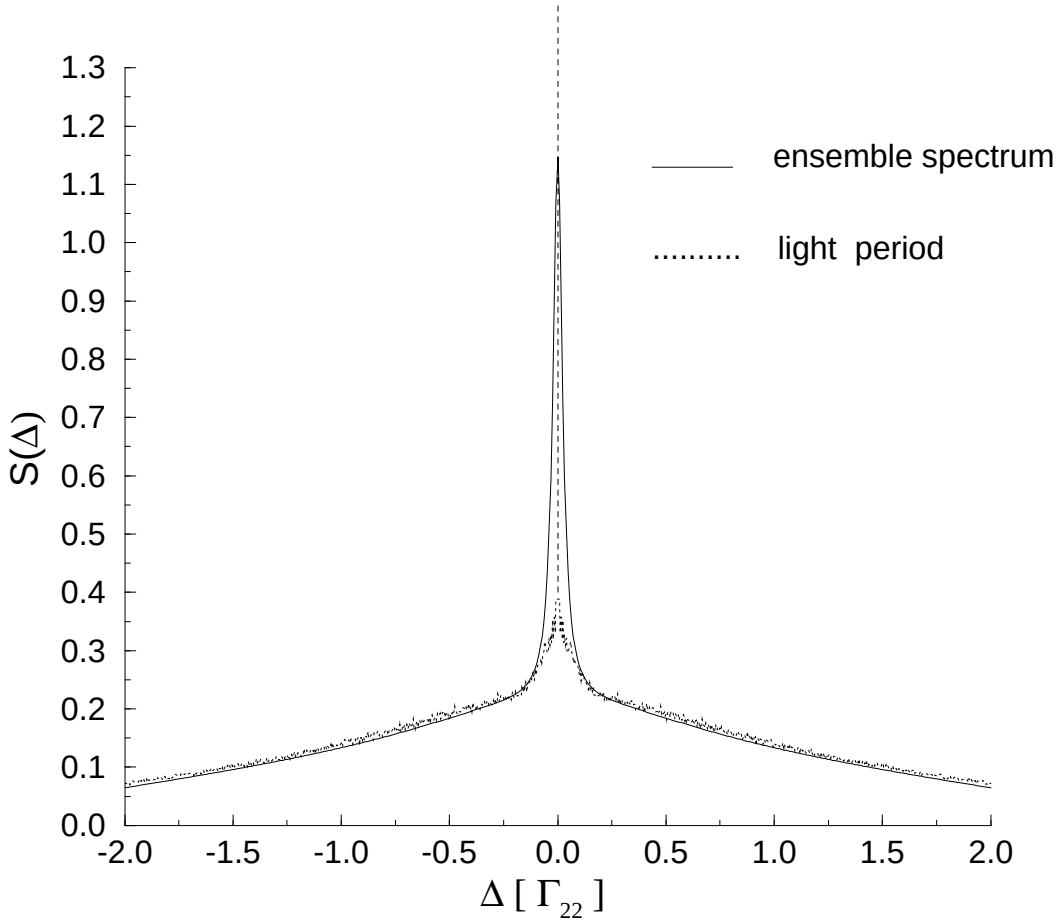
2.0
Δ [Γ22]


spectral analyzer
broadband counter (trigger)
atom


1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
S(Δ)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
Δ [Γ22]
ensemble spectrum
light period